Three-Dimensional Rayleigh-Bénard Convection of a Rarefied Gas: DSMC and Navier-Stokes Calculations

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Abstract. The three-dimensional Rayleigh-Bénard convection of a rarefied gas is studied numerically by using DSMC and Navier-Stokes finite difference methods. We present the results obtained in a three-dimensional box with an aspect ratio $A=L_x:L_y:L_z$ at a fixed wall temperature ratio $r=T_c/T_h=0.1$. In general, the three-dimensional results confirm the validity of the zone of convection obtained in the previous author's two-dimensional considerations [1,2]. A detailed analysis has been performed for Knudsen number Kn=0.02 and A=2:2:1, A=3:3:1, and A= 4:4:1 and different Froude numbers ranged within the zone of convection. As result, a variety of different stable convection patterns in form of rolls and squares has been obtained. For the lowest Knudsen numbers computed, Kn=0.001 and Kn=0.002 , Froude number Fr= 1.0, and a fixed aspect ratio A=2:2:1, an irregular (chaotic) flow in form of unstable polygonal patterns has been observed.

INTRODUCTION

The formation and development of convection flows in a fluid confined between two horizontal parallel plates with the bottom plate heated from below is a classical problem known as the Rayleigh-Bénard problem. In our previous papers [1, 2] we have studied the formation of convection patterns in the Rayleigh-Bénard (RB) flow of a rarefied gas in a rectangular two-dimensional domain by using two different numerical approaches: particle simulation by the DSMC method and Navier-Stokes finite difference (FD) calculations. The calculations have been performed within a range of Knudsen number Kn = 0.001-0.04 and Froude number $Fr=0.5\text{-}1.5\times10^3$ and a fixed temperature ratio r=0.1. We have observed a variety of possible final states (attractors), namely: pure heat conduction, stable vortex roll convection, periodic, wavy, and chaotic regimes.

In the present paper we extend the study of the problem to convection gas flows in a three-dimensional box. The low Knudsen numbers allow again the problem to be investigated by using two numerical approaches: DSMC method (particle approach) and finite difference method (continuum approach based on the model of compressible viscous heat conducting gas with state-dependent transport coefficients). Using the DSMC method, the three-dimensional convection of a rarefied gas has been investigated by Watanabe [3] for the case of a hypothetical value of the gravitational acceleration (the Froude number in non-dimensional formulation) so as to minimize the density variation in the pure heat conduction state. The same approach, imitating the conditions of the Boussinesq approximation (valid for continuum fluid dynamics), has been used previously by Garcia *et al.* [4] and Watanabe *et al.* [5] for the two-dimensional case of convection in rarefied gas. In our calculations, the governing non-dimensional parameter Fr was varied freely so strongly stratified states could be investigated. This idea was proposed by Stefanov and Cercignani [6] and used by Sone *et. al.* [7], Stefanov *et. al.* [1,2] for a detailed investigation of the two-dimensional Rayleygh-Bénard problem of a rarefied gas. In the present paper we follow that second approach and investigate the three-dimensional RB flow for a set of Kn and Fr at fixed temperature ratio r=0.1. The dependence of the pattern formation on the aspect ratio $A = L_x:L_y:L_z$ is also studied. The most detailed analysis is performed for Kn=0.02, Fr=3.0 and aspect ratios A=2:2:1, A=3:3:1 and A= 4:4:1. For the same Kn=0.02 and aspect ratios A=2.0 and A=3.0 the calculation are performed for Fr=1.5, Fr=3.0 and Fr=7.0. The next computations have been performed for sufficiently low Knudsen numbers Kn=0.002 and Kn=0.001, where one can expect development of more complicated flow regimes, as was discovered in [1,2] for the two-dimensional RB flow.

CP762, *Rarefied Gas Dynamics: 24th International Symposium,* edited by M. Capitelli

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
13 JUL 2005	**N/A**	**-**

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Three-Dimensional Rayleigh-Bénard Convection of a Rarefied Gas: DSMC and Navier-Stokes Calculations	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Institute of Mechanics, BASci., Acad. G. Bonchev Str., Block. 4, 1113 Sofia Bulgaria**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES
See also ADM001792, International Symposium on Rarefied Gas Dynamics (24th) Held in Monopoli (Bari), Italy on 10-16 July 2004.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**UU**	**6**	

In general, the analysis of the obtained results for the three-dimensional Rayleigh-Bénard flow show that the zone of governing parameters, in which a transition from pure heat conduction to the regime of convection takes place, is in good agreement with the zone delineated by the two-dimensional calculations [1]. A chaotic convection in form of different unstable polygonal patterns has been obtained within the range of Knudsen numbers Kn=0.001-0.002 and a Froude number around Fr=1.0-1.1. For larger Kn and Fr we have observed a variety of stable structures in form of roll or square patterns.

Problem Formulation And Computational Considerations

The three-dimensional Rayleigh-Bénard problem for a rarefied gas treats a monatomic simple gas with average number density n_0 studied in a rectangular computational domain $D(L_x x L_y x L_z)$ i.e. with an aspect ratio $A=L_x/L_z:L_y/L_z:L_z/L_z$. The domain is confined in the vertical z-direction by two diffusely reflecting horizontal walls (the lower wall temperature is greater than the upper one, $T_h > T_c$) and a periodic boundary condition is implemented in the horizontal x- and y-directions at vertical planes at mutual distances L_x and L_y. A constant acceleration $\mathbf{g}=(g_x,g_y,g_z)=(0,0,-g)$ acts on the gas in each point of the computational domain. A hard sphere molecular model is employed in the simulation of binary collisions. The governing nondimensional parameters are the Knudsen number $Kn=\ell_0/L_z$, the Froude number $Fr=V_{th}^2/gL_z$, and the temperature ratio $r=T_h/T_c$, where ℓ_0 is mean free path in a "hard sphere" gas with density n_0, and V_{th} is the most probable molecular velocity in equilibrium gas with temperature T_h. In our consideration all variables are normalized by using the following scales: for density, $\rho_0=mn_0$ (m is the molecular mass); for velocity, V_{th}; for length, the distance L_z; for time, $t_0=L_z/V_{th}$; for temperature, T_h.

The time evolution of this system when starting from a certain initial state has been studied by means of the two approaches discussed in the introduction: molecular and continuum.

The DSMC technique uses a finite number of model particles that move and collide in the three-dimensional space domain D to perform a direct simulation of the molecular gas dynamics. The algorithm follows the basic steps of the ``No Time Counter'' scheme suggested by Bird [8]. A uniform rectangular basic grid with $N_x x N_y x N_z$ cells covers the computational domain. Within every time step each basic cell is subdivided dynamically into subcells in order to meet the special resolution requirements; the size of a subcell is less than the local mean free path. In this way, only the information about the basic grid is kept permanently in the computer memory. The sampling is conducted on a coarser grid with larger cells containing a group of basic cells. This multilevel grid scheme allows a correct calculation of the molecular process on an adaptive fine grid and at the same time provides a meaningful sample size of the instantaneous macroscopic variables by averaging simultaneously over a group of cells. For example, for Kn=0.02 and A=2:2:1 a grid with 100x100x50 basic cells is used; while for Kn=0.02 and A=4:4:1 – 200x200x50. For the computed lower Kn=0.002 the grid at A=2:2:1 is with 200x200x100 basic cells. The instantaneous fields are sampled by time averaging over 500 time steps Δt (Δt is less than mean collision time) Finally, the obtained three-dimensional instantaneous macroscopic fields are processed by a simple average filter in order to remove the high-frequency statistical fluctuations from the simulation results. Depending on the Knudsen number and the aspect ratio A the total number of model particles varies from $5x10^6$ to $32x10^6$.

The 3D finite difference (FD) calculations of the continuum model based on the Navier-Stokes equations for a compressible viscous gas with state dependent transport coefficients (see [1]) are performed by using an implicit conservative finite difference (second order in space and first order in time) scheme with inner iteration process within each time step. During each iteration a 7-bandmatrix linear equation system obtained for each macroscopic variable is solved by using a generalized conjugate gradient (GCG) method. The iteration error is chosen to be not larger than 10^{-10} – 10^{-11} depending on the chosen computational parameters of the scheme. The size of the rectangular uniform computational grid depends on the Knudsen number and the aspect ratio A. For the most difficult cases, Kn=0.002 and Kn=0.001 at fixed aspect ratio A=2.0, a grid with 200x200x100 nodes is used. For the larger Kn=0.02 the calculations are performed on grids 100x100x50 , 150x150x50, and 200x200x50 for aspect ratios A=2.0, A=3.0, and A=4.0, respectively.

Numerical Results

We illustrate the obtained results using a limited set of the computational data. In our previous works [1,2] we have shown that the two-dimensional calculations of the RB flow, performed by using both molecular and continuum approach for the range of the governing parameters mentioned in the introduction, exhibited a qualitative and quantitative similarity of the obtained convective flows. That is why, here our main goal is not to present a detailed comparison of both model calculations for the three-dimensional case of RB flow but to use each of the two

models where it is more effective in order to cover a wider range of the parameters where new interesting convection phenomena might exist. A rough preliminary comparative analysis has convinced us that we could not expect great surprises and both models should give similar results within the studied range of the parameters. This work is in progress and a more detailed discussion on the comparison of the two models in the three-dimensional case of the RB convection will be given in a separate paper. Here we follow the line of presenting our results for a set of calculations performed by using the DSMC simulations for Kn=0.02 and various Fr and aspect ratios where the particle method was more effective than the finite difference computations. In the cases with a smaller Knudsen number, Kn=0.002 and 0.001, the FD method was considerably more effective because it turned out possible to obtain a quantitatively correct results on sufficiently coarser grid than a grid that meets the computational requirements of the DSMC method. Thus, the results presented here for the chaotic convection at Kn=0.002 and Fr=1.0 were computed by using the FD method. This case was run by DSMC within the initial part of the transient period where the results were similar to those obtained by FD. For the comparative analysis in this case, the DSMC calculations will be continued beyond the transient period.

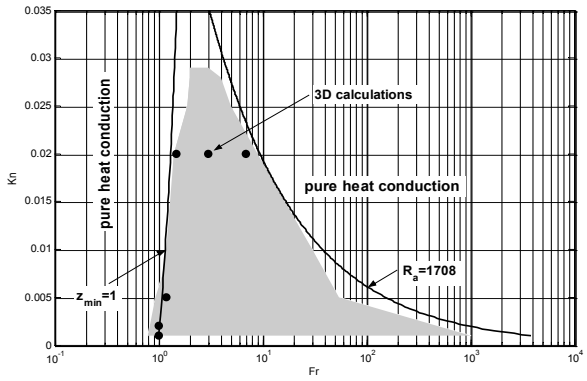
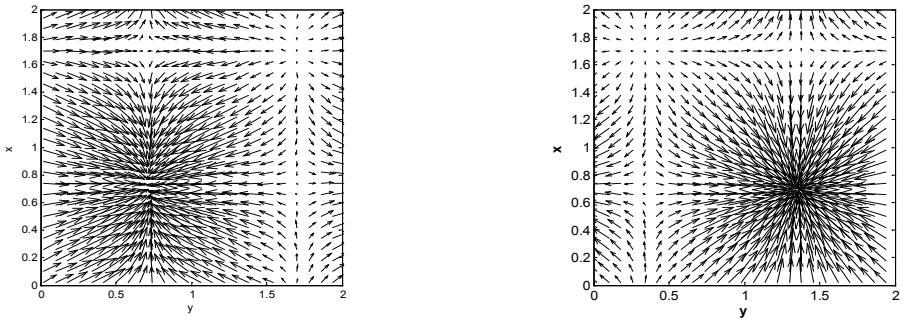


FIGURE 1. The zone of convection and the points of the three-dimensional computations: the analytical conditions for the left and right boundaries of the zone of convection [1].are given with solid lines, the gray shaded zone illustrates the two-dimensional calculations [1,2], the three-dimensional calculations are given with filled circles.

Figure 1 shows the points (filled circles) of the three-dimensional calculations in a coordinate system of Fr and Kn numbers (the temperature ratio is fixed r=0.1). The gray shaded polygon illustrates the zone of convection obtained from the two-dimensional calculations [1]. The analytical conditions for the left and right boundaries of the zone of convection (eqs. (15) and (16) in [1]) are shown by solid lines. Additionally, several 3D calculations have been performed for points outside of the delineated zone of convection but close enough to its boundaries. In general, these 3D-runs, performed by using DSMC method for Kn=0.02 and Kn=0.01, confirmed the two-dimensional results [1] obtained for the boundaries of the zone of convection.

Figures 2 and 3 illustrate the convection patterns for fixed Kn=0.02 and A=2.0 at Fr=1.5 (a) (the left side



(a) (b)

FIGURE 2. Velocity vector field in xy-plane at z=0.9for Kn=0.02, A=2, and Fr=1.5 (a) , Fr=7.0 (b).

of the convection zone where gravity prevails against the temperature gradient action) and at Fr=7.0 (the right side, where the temperature gradient is dominating). The "view form above" at z=0.9 (Fig. 2) showed that in both cases the convection flow is organized as an asymmetrically positioned single square cell with a single sink point (the focal point of the velocity vectors). Figure 3 shows the similar vortex configuration in a vertical plane section at x=0.5 in cases (a) and (b) as defined in Figure 2. From the figure one can see that the vortex center is shifted up with the increase of the Froude number.

(a) (b)

FIGURE 3. Velocity vector field in yz-plane at x=0.5for Fr=1.5 (a) and Fr =7.0 (b)

Figures 4 and 5 show the flow patterns for different aspect ratios A=2, A=3, and A=4 at Kn=0.02 and Fr=3.0.

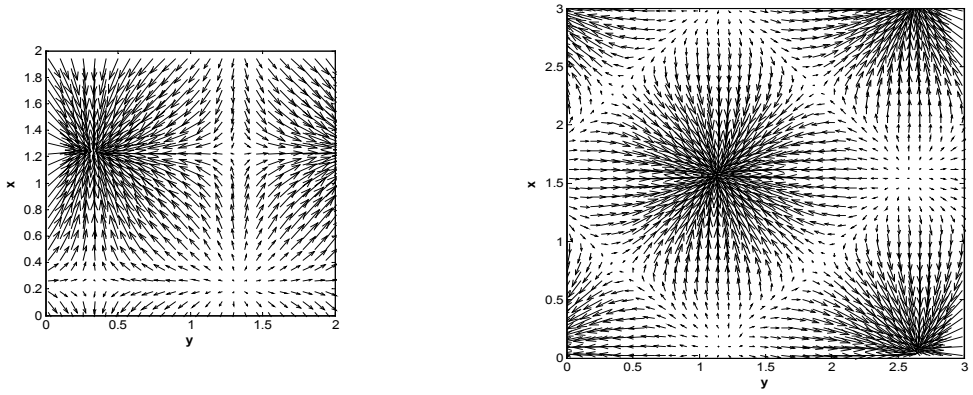


FIGURE 4. Velocity vector field in xy-plane at z=0.9 for Kn=0.02 , Fr=3.0 and aspect ratios A=2 (left), A=3 (right)

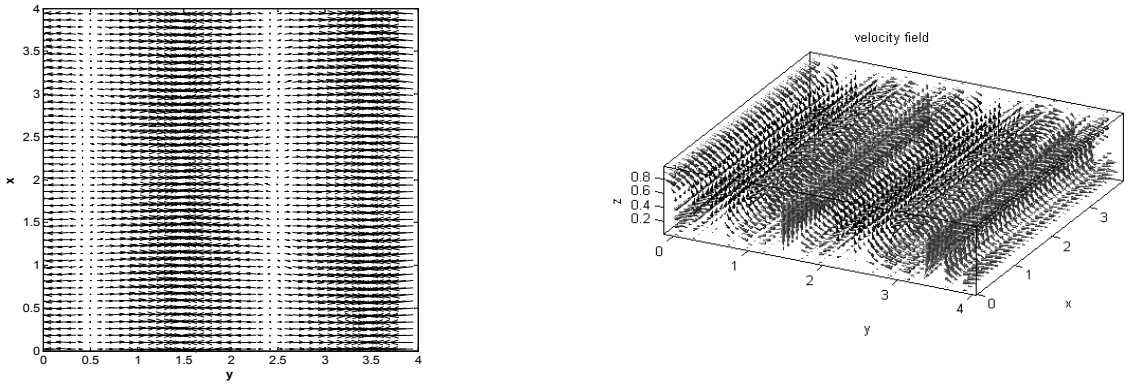


FIGURE 5. Velocity vector field in xy-plane at z=0.9 (left) and 3D velocity vector plot for Kn=0.02 , Fr=3.0, A=4.0.

The flow pattern for A=2 is again a single square cell. For A=3 the result is different – inclined square cells with a size equal to the pattern size in the case A=2. The picture for A=4 is drastically changed: the flow patterns are stable four rolls (Fig. 5, (right)) with hardly seen in Figure 5 (left) variable thickness chess positioned. This effect can be seen from the density plot at the middle plane z=0.5 in Fig. 6 (left). In order to keep this configuration stable the velocity field is structured in a complicated way illustrated in Fig.(6) (right) with the xy-velocity field at z=0.5. Here one can observe a stable low intensity secondary flow in xy- directions.

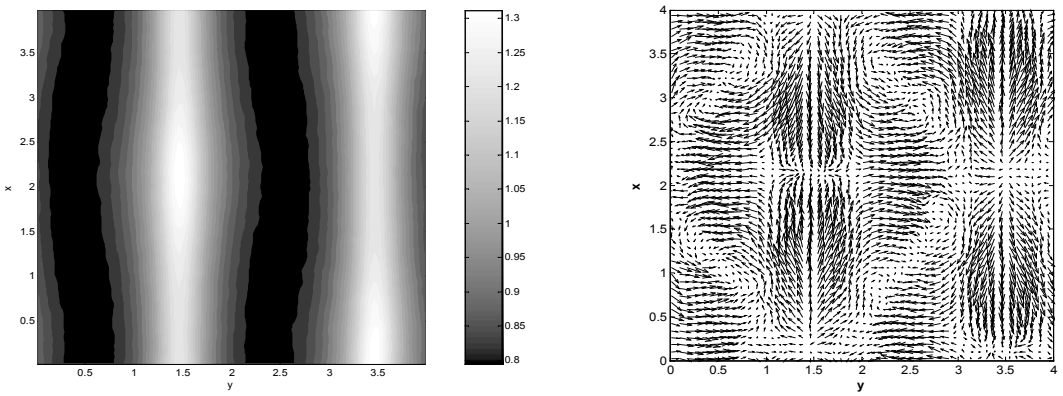
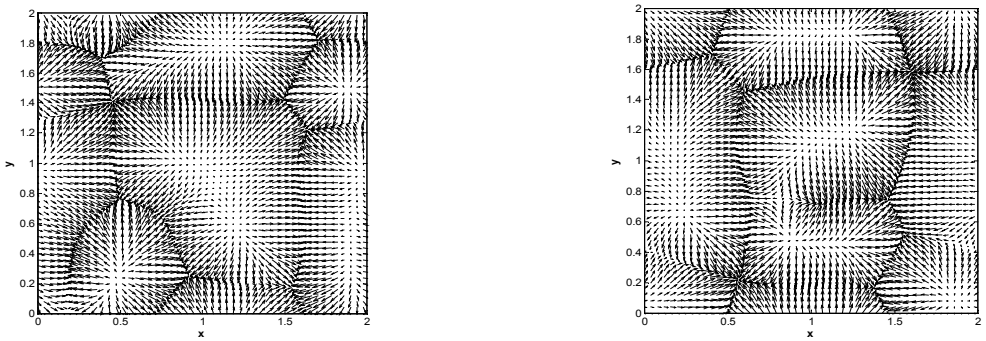


FIGURE 6. The density field at z=0.5 (left) and the 3D velocity vector plot (right) for Kn=0.02, A=4.

The analysis of the flow patterns obtained by DSMC simulations for Kn=0.02 leads to following two conclusions. First, the flow configuration depends strongly on the boundary conditions and the aspect ratio. Thus, for the small aspect ratio A=2 we have a single square cell for all magnitudes of Fr ranged within the zone of convection. For A=3 the patterns are the same in form and size but are inclined. Similar inclined patterns have obtained by Watanabe [3] for odd aspect ratios. This can be explained with the link between the periodicity boundary conditions and the odd aspect ratio. Second, there are long ranged correlations which are cut-off in the small aspect ratio computations. This conclusion is supported by the results shown in figures 5 and 6. The case with A=4 shows that the larger computational box allows four roll configuration; this is not observed in the cases with A=2.0 and A=3.0.

Figures 7 (a) – (f) present a case of chaotic Rayleigh-Bénard convection at Kn=0.002, Fr=1.0, and r=0.1, obtained by using Navier-Stokes calculations. The series of snapshots taken at different times after the end of the transient period illustrates the time evolution of the convection patterns within a period of about 100 units in the chosen time scale. The times are selected in a way that the xy-velocity vector fields at a fixed z=0.9 (close to the cold wall) show a variety of typical flow patterns. Most of them are in the form of unstable polygonal configurations interacting with each other in a complicated way. In the figures the narrow stripes with gathering arrows of the velocity vectors delineate the edges of the polygons where the cold flux goes down from the cold (top) to the hot (bottom) wall. Within a wide area inside the polygons the flux is directed up. The size of the configurations varies from small flow patterns (Fig. 7 (c)) less than 1/10 of the computational box size to large ones (Fig. 7 (e)) comparable to it.



(a) (b)

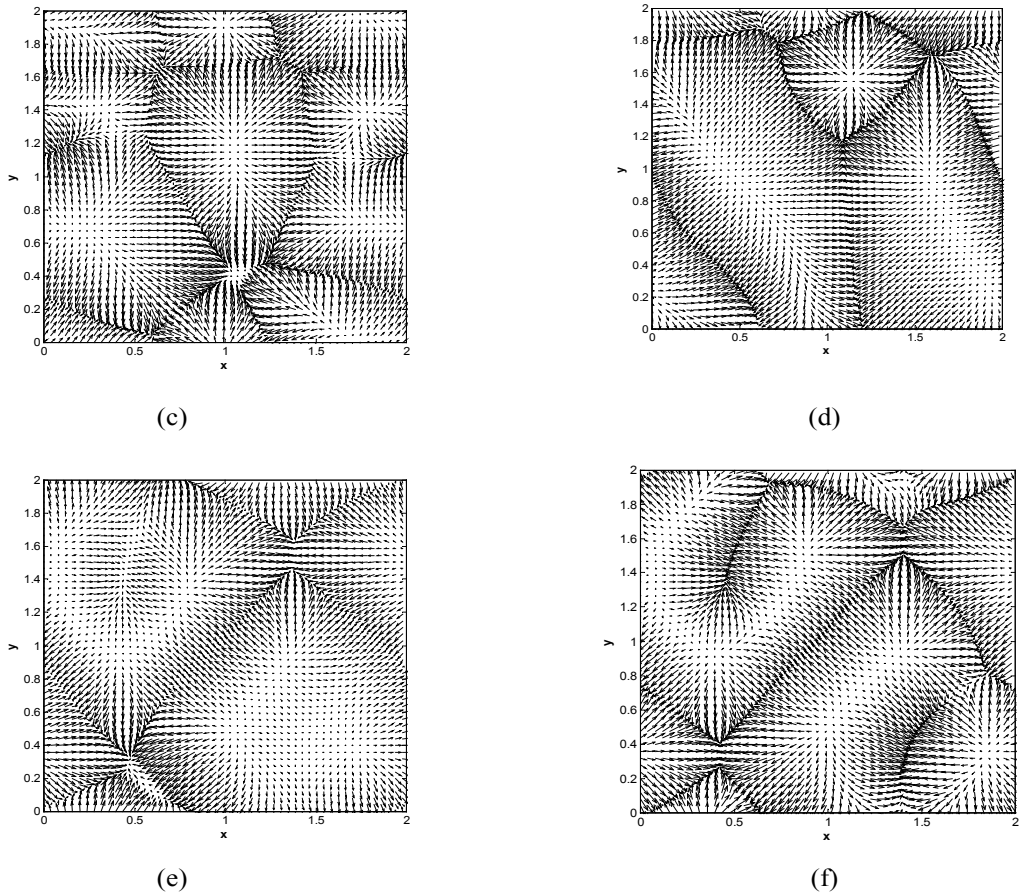


FIGURE 7. Instantaneous velocity vector filed for Kn=0.002, Fr=1, A=2 at different times: (a) t=200.0; (b) t=220.0; (c) t=235.0; (d) t=260.0; (e) t=280.0; (f) t= 300.0.

ACKNOWLEDGMENTS

The research described in this paper was supported by MURST of Italy and the Bulgarian Ministry of Education and Sciences.

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